

PERFORMANCE ANALYSIS OF DIVIDING WALL COLUMN MODEL FOR FRACTIONATION OF OLEOCHEMICAL FATTY ACID

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ABSTRACT

Fractionation process of oleochemical products in Malaysia normally uses conventional distillation columns (CDC). Due to the considerable amount of energy used in the separation process, there is a need to have an intensified process. Dividing wall column (DWC) is an attractive option which offers big advantages with reduced cost and energy consumption. However, research on its feasibility for oleochemical fractionation is scarce. In this article, we conducted a model-based performance analysis of DWC for oleochemical fatty acid fractionation. The model was designed and simulated using a customised four column configurations in Aspen Plus. A step-by-step design procedure was introduced to aid the model development. Economic and environmental assessment was performed and compared with conventional distillation columns. Hydraulic analysis of several packing type was also performed to gain insights on the column hydrodynamic behaviour. Our result shows that the major economic advantage is in the operating cost with savings of up to 16.9% and 10.2% on cooling and heating utilities, respectively while reduces 10.2% of CO₂ emissions. Overall, our study shows the feasibility of fractionating fatty acids in oleochemical industry using DWC. Such assessment is important to assess its feasibility especially during the early stage of technology development prior to industrial implementation.

Keywords: process modelling, dividing wall column, oleochemical fatty acid.

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INTRODUCTION

Distillation is one of the most common separation methods, as it is widely understood and used to a great extent for separating liquid mixtures. Although its thermodynamic efficiency is low, the ease and confidence in operation makes distillation one of the most preferred separation methods (Sangal *et al.*, 2013). However, distillation columns

(DC) consume a substantial part of the entire energy requirement for chemical industry. The United States Department of Energy reported that there are more than 40 000 DC in North America alone, and these columns are estimated to consume 40% of the total energy to operate plants in the refining and bulk chemical industries (Demire, 2013). Therefore, reducing this energy consumption could significantly achieve overall plant energy savings and increase the plant profitability. This motivates researchers to focus on developing and improving the efficiency of distillation processes. One of them is the dividing wall column (DWC). Over the years, DWC has attracted many studies and has been successfully implemented in process industries, especially for separating ternary mixtures. It is a

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promising energy saving alternative for separating multi-component mixtures of hydrocarbons, alcohols, aldehydes, ketones, acetals, amines and others (Serra *et al.*, 1999; Yildirim *et al.*, 2011). In recent developments, application of DWC has been extended to other separation processes such as azeotropic, extractive and reactive distillation (Kaur and Sangal, 2017; Weinfeld *et al.*, 2018). However, application of DWC has its own limitations due to the challenges in design, simulation, operation and control (Dejanović *et al.*, 2010; Yildirim *et al.*, 2011). Nevertheless, it is predicted that future implementations of DWC technology will be in developing countries with emerging markets rather than in countries with established distillation networks (Yildirim *et al.*, 2011).

In 2017 and 2018, Malaysian crude palm oil (CPO) production recorded more than 19.8 million tonnes (MPOB, 2019). Oleochemical industry in Malaysia is now becoming one of the largest in the world, with about 20% of the world's capacity. From our survey of 17 oleochemical plants in Malaysia, it is found that all of them employ series of typical DC for fractionation of its oleochemical products. Faesler *et al.* (2007) also mentioned a few applications of DWC in the oleochemical sector due to the limited familiarity, higher requirements on operation, potential corrosion problems and limited flexibility. Considering DWC benefits and implementations in the US and Europe, especially for chemical industries, application of DWC to oleochemical industries in Malaysia offers huge opportunity which will further leverage the oleochemical industry in Malaysia. This is aligned with the Roundtable on Sustainable Palm Oil (RSPO) and Malaysian Sustainable Palm Oil (MSPO) initiatives as the well as Malaysia National Key Economic Area (NKEA) agenda to improve energy efficiency and to ensure sustainability for improved productivity of palm oil industry. However, there are few studies on DWC applications for oleochemical fractionation processes. Among these few, Illner and Othman (2014) and Othman *et al.* (2015) simulated a four-column configuration for oleochemical fatty acid (FA) fractionation. However, these articles

focus on general modelling procedure and design of experiment-based optimisation, and do not evaluate the feasibility of DWC. Therefore, in this article, we introduce a more detailed design procedure of DWC as well as model-based feasibility and comparison study of DWC for oleochemical applications. Our case study will focus on FA fractionation.

Fractionation of FA cuts from refined, bleached and deodourised (RBD) palm kernel oil (PKO) is typically done through thermal separation using DC. The main FA cuts from RBD PKO that need to be fractionated are: C6-C10 (pre-cut, PC), C12 (light cut, LC), C14 (middle cut, MC) and C16-C18 (heavy cut, HC). Table 1 shows the common FA chains and their physical properties. Due to the distinctive boiling point differences, it is interesting to analyse the possibility of fractionating the cuts using DWC. Typically, with inclusion of residues such as triglycerides (TG), four direct sequence DC can be used to fractionate all the FA cuts as shown in Figure 1a. Alternatively, an intensified process is possible by using two DWC in series namely DWC1 and DWC2, as shown in Figure 1b. The aim of this work was to investigate the feasibility of modelling such a process and to assess its performance. In doing that, we proposed a design procedure to model and simulate the process in Aspen Plus using a customised four-column configurations. A four-column configuration is a more realistic approach to represent each four internal sections of DWC. Based on the model, we analysed and compared its economic and environmental performance as well as the hydrodynamic and thermal analysis. We believe such a study is important during early stage of technology development to gain stakeholders confidence for utilising DWC in their plans.

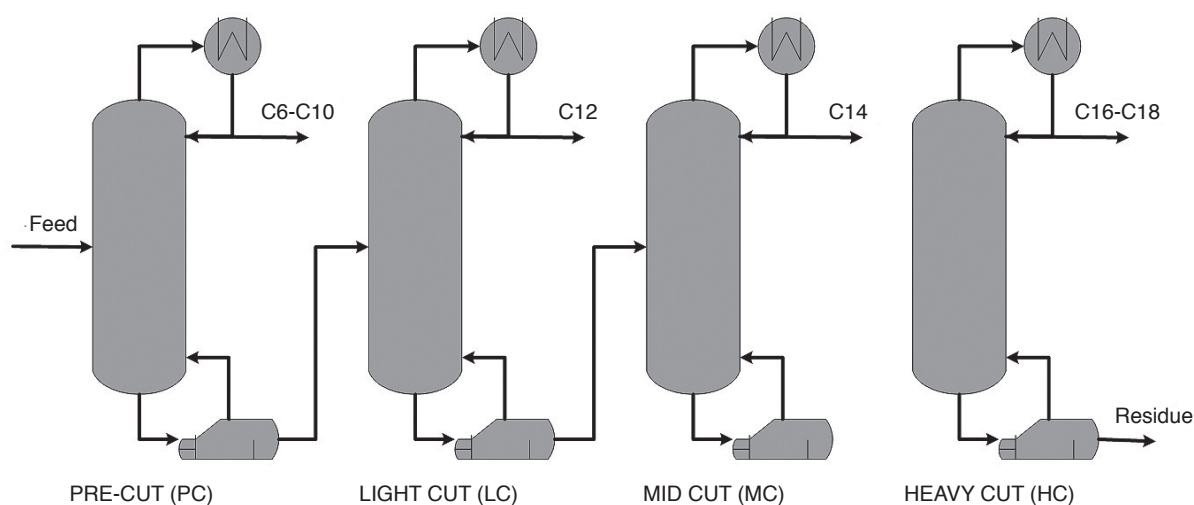
METHODOLOGY

A hierarchical approach was proposed for conducting the design and performance analysis as shown in Figure 2. The approach was divided into four parts. The first part was the problem definition. The main objective was to analyse the performance

TABLE 1. COMMON FATTY ACIDS IN OLEOCHEMICAL INDUSTRIES AND THEIR PHYSICAL PROPERTIES

Component	Cuts	Molecular weight	T _{BP} (°C)	Dipole moment (debye)
(C6) Caproic acid, C ₆ H ₁₂ O ₂	Pre-cut (PC)	116.16	205.7	1.57092
(C8) Caprylic acid, C ₈ H ₁₆ O ₂	Pre-cut (PC)	144.21	239.7	1.69983
(C10) Capric acid, C ₁₀ H ₂₀ O ₂	Pre-cut (PC)	172.27	270.0	1.67884
(C12) Lauric acid, C ₁₂ H ₂₄ O ₂	Light cut (LC)	200.32	298.7	1.63987
(C14) Myristic acid, C ₁₄ H ₂₈ O ₂	Middle cut (MC)	228.38	326.2	1.67884
(C16) Palmitic acid, C ₁₆ H ₃₂ O ₂	Heavy cut (HC)	256.43	350.0	1.7388
(C18:1) Oleic acid, C ₁₈ H ₃₄ O ₂	Heavy cut (HC)	280.45	354.9	1.21716
(C18:2) Linoleic acid, C ₁₈ H ₃₂ O ₂	Heavy cut (HC)	282.47	359.9	1.43901
(C18) Stearic acid, C ₁₈ H ₃₆ O ₂	Heavy cut (HC)	284.483	374.0	1.66985

(a)



(b)

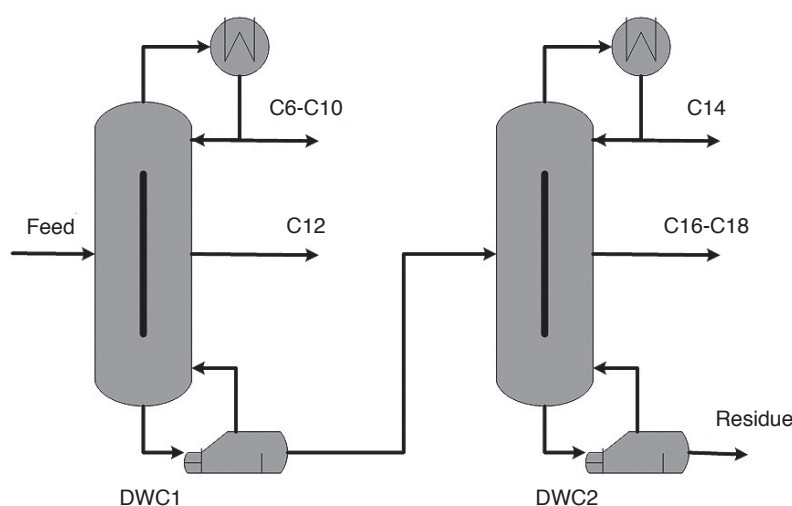


Figure 1. Process configuration for four-product fractionation using (a) distillation columns (DC) and (b) dividing-wall columns (DWC).

of DWC for oleochemical FA fractionation. Aspen Plus V9 was used to model and simulate the process. The feed information used in this work, obtained from our industrial partner, is shown in Table 2. The desired product specifications to be achieved were 99 wt% of C6-C10, C12, C14 and C16-C18. Apart from the FA cuts, residue such as TG was also included in the feed; it was represented by a pseudo-component: TAGPOLN with molecular weight of 855.38 and boiling point temperature of 534.2°C. Note that, to prevent product degradation, the column reboiler temperatures were operated below 270°C and therefore all columns in FA fractionation were operated under vacuum between 10 mbar to 40 mbar.

Modelling

The second part focused on the model development. Three models were developed in this work, namely, Case 1, Case 2 and Case 3, each with increasing complexity (Figure 2). Case 1 and Case 2 were based on a typical four direct-sequence DC, in which all products are at the distillate streams. Case 1 was modelled based on shortcut method using four DSTWU blocks. DSTWU model uses Winn method to estimate minimum number of stages, Underwood method to calculate minimum reflux ratio and Gilliland method to estimate number of stages at the chosen reflux ratio. It is assumed that relative volatilities and molar over flow are constant. The

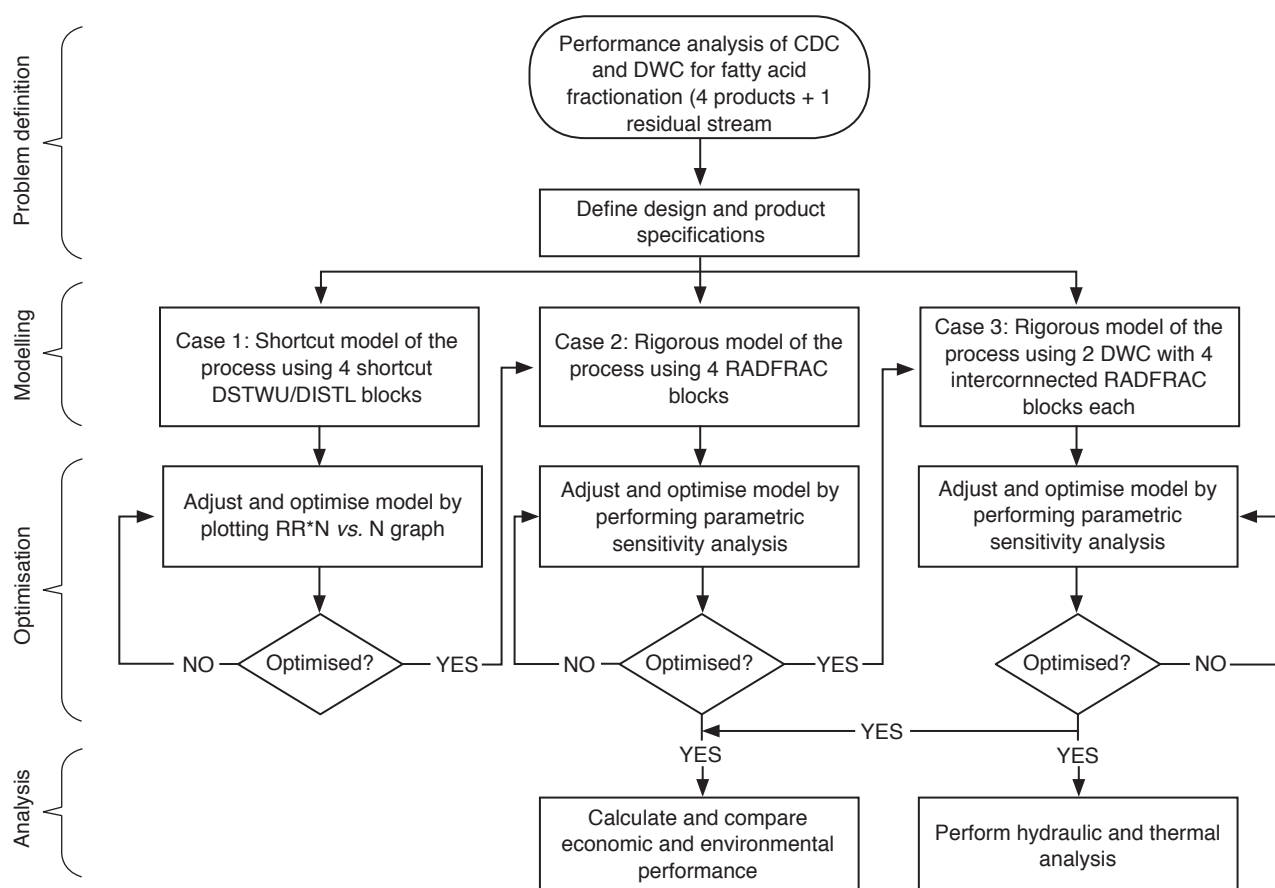


Figure 2. Four-part approach for performance analysis adopted in this work.

TABLE 2. FATTY ACIDS FEED INFORMATION OBTAINED FROM OUR INDUSTRY PARTNER

Feed flow rate (kg hr ⁻¹)	9 167
Feed temperature (°C)	30
Feed pressure (bar)	1
Component	Mole fraction
Caproic acid (C ₆ H ₁₂ O ₂)	0.0012
Caprylic acid (C ₈ H ₁₆ O ₂)	0.033
Capric acid (C ₁₀ H ₂₀ O ₂)	0.034
Lauric acid (C ₁₂ H ₂₄ O ₂)	0.474
Myristic acid (C ₁₄ H ₂₈ O ₂)	0.162
Palmitic acid (C ₁₆ H ₃₂ O ₂)	0.079
Oleic acid (C ₁₈ H ₃₄ O ₂)	0.1562
Linoleic acid (C ₁₈ H ₃₂ O ₂)	0.026
Stearic acid (C ₁₈ H ₃₆ O ₂)	0.0188
Triglycerides (C ₅₅ H ₉₈ O ₆)	0.0099

results from Case 1 were used for initial estimation in modelling of Case 2. Case 2 was modelled using four direct-sequence RADFRAC blocks connected in series namely PC, LC, MC and HC columns where the distillate product were C6-C10, C12, C14 and C16-C18, respectively. RADFRAC involves rigorous calculations assuming equilibrium stages, which is commonly used for distillation systems. The results from Case 2 were then used as initial design

parameters for simulating Case 3. Case 3 involved two DWC, *i.e.* DWC1 and DWC2. The distillate and middle product for DWC1 were C6-C10 and C12 while distillate and middle product for DWC2 were C14 and C16-C18. The modelling approach for Case 3 was also based on equilibrium stage. Note that DWC block was not available in Aspen Plus and need to be customised. Therefore, modelling a DWC was not straightforward compared to a DC.

In Case 1 using DSTWU block, one needs to specify number of stages or reflux ratio as an initial guess, light key (LK) and heavy key (HK) components, and their recoveries. The LK recovery is the least volatile component enriched in the distillate stream whereas HK is the most volatile component enriched in the bottom stream. C10 and C12 were selected as the LK and HK for PC column; C12 and C14 were the LK and HK for LC column; C14 and C16 were the LK and HK for MC column; and C16 and TG were the LK and HK for HC column. Recovery values for both LK and HK were based at the distillate stream. For all columns, LK recovery was 0.99 while HK recovery was 0.01. The results from Case 1 such as minimum number of stages, reflux ratio, number of stages at chosen reflux ratio and feed stage would be used as initial estimates for input parameters for Case 2.

Thermodynamic method. For the determination of thermodynamic and hydrodynamic properties, different property packages can be used to estimate the required parameters, according to the case under study. As shown in Table 1, based on the dipole moment values, fatty acids are polar components. Activity coefficient models are suggested for non-electrolyte polar components and operation less than 10 bar. Such models are non-random two-liquid (NRTL) model, universal quasichemical (UNIQUAC) and its variants. An effort has been made to compare predictions by UNIQUAC and NRTL with the National Institute of Standards and Technology (NIST) experimental data, available within Aspen Plus. The Txy plots for NRTL and UNIQUAC models for lauric acid (C12) and myristic acid (C14) were considered, and the comparative results are shown in Figure 3. Based on the best fit to NIST data, NRTL model was chosen and employed in this work.

DWC design. Generally, reasons for not utilising DWC in industries are due to its complexity, lack of experience and difficulty to control (Dejanovic *et al.*, 2010). Nevertheless, with the advancement of process simulators equipped with state-of-the-art computational techniques, comprehensive thermodynamic packages and large component libraries, process simulators today provide reliable results for process design and operation of DWC. A sequential-modular modelling is often used for simulating DWC; however, DWC block is currently not available in commercial process simulators. Hence, two or more distillation blocks have to be arranged to represent the unique structure of DWC. Most often, two-column configuration (Premkumar and Rangaiah, 2009; Delgado-Delgado *et al.*, 2012; Kiss and Ignat, 2012) is employed for rigorous simulation of a DWC. However, four-column

configuration is better to represent the four internal sections of a DWC as it offers flexibility in sizing the column sections and suitability for dynamic simulation and control study (Dejanovic *et al.*, 2011).

A four-column configuration, shown in Figure 4, was employed in the present study. Since a unique block was used to represent each of the four internal sections of DWC, the four-column configuration could lead to better modelling of column internal behaviour such as hydraulics and thermal profile as well as relatively more accurate cost estimation. Sections A, B, C and D in Figure 4 represent the rectifying, pre-fractionator, middle and stripping sections of DWC, respectively. The RADFRAC block for sections A and D was set to have a condenser and reboiler respectively, whereas both sections B and C have neither a condenser nor a reboiler. By using this set-up, degrees of freedom (DOF) was reduced compared to a typical column with a reboiler and a condenser, which usually has DOF of two. Section A had only one DOF, where the reflux ratio was selected and specified. Sections B and C had no DOF, and so no specification to be given. Section D had one DOF, for which reboiler duty was selected and specified.

In addition, DWC set-up in Figure 4 had two DOF, which were liquid (M1) and vapour (M2) split. Initially, vapour and liquids split were set equally. In reality, vapour split is difficult to control whereas liquid split can be manipulated using magnetic or pneumatic valve. The other advantage of a four-column configuration is that it provides better insights of the column performance as well as capable of conducting thermal and hydrodynamic analysis. But such a model has convergence issues. A much simpler and straightforward approach to DWC column design was introduced by Becker *et al.* (2001). Based on our experience, we extended Becker's approach to facilitate the initial design of

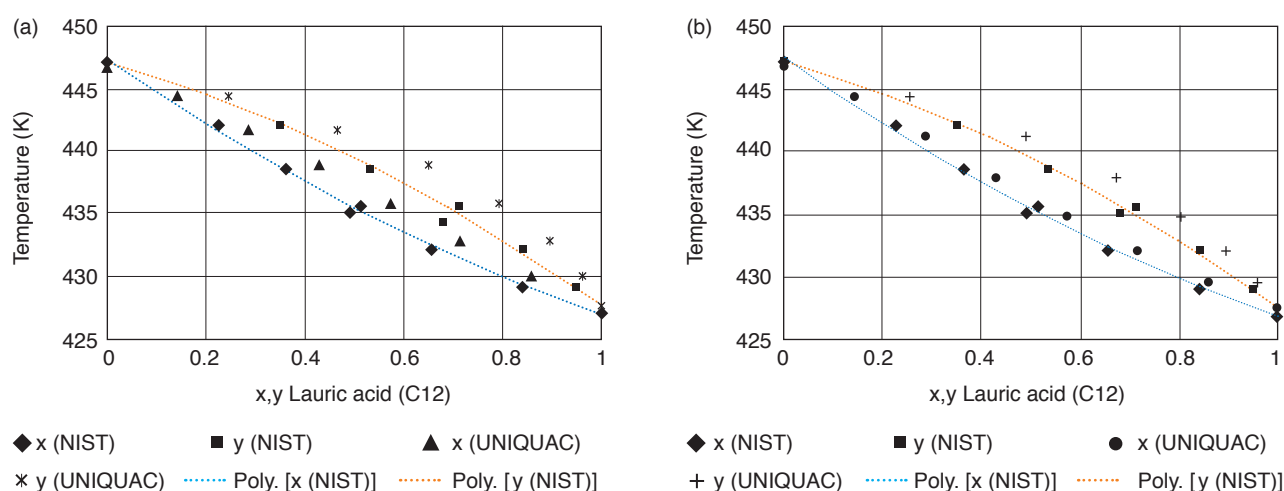


Figure 3. Txy diagram for C12/C14 between National Institute of Standards and Technology (NIST) data and universal quasichemical (UNIQUAC) predictions (left plot), and between NIST data and non-random two-liquid (NRTL) model predictions (right plot). The dotted line is the polynomial curve for the NIST data.

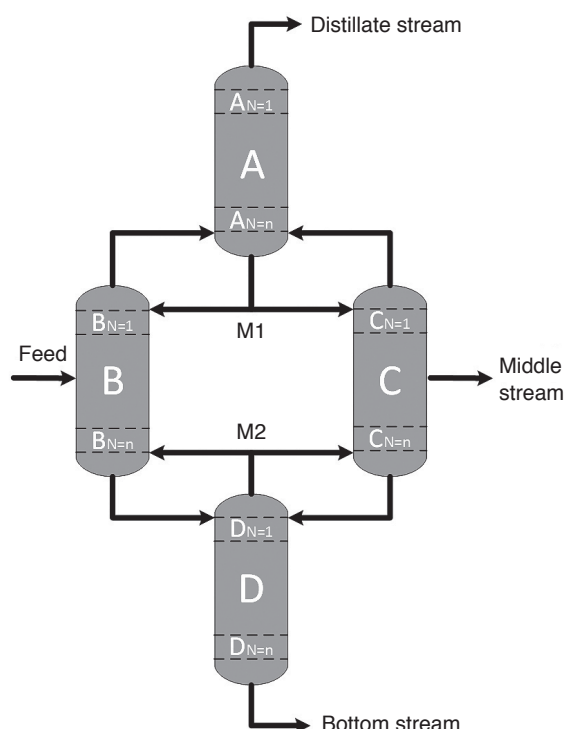


Figure 4. Four-column configuration for dividing wall columns (DWC) simulation.

DWC. Note that, in this approach ternary mixtures were considered with no pressure drop and tray/packing design. The approach can be adopted for other process as well. The improvised approach was as follows:

1. Model and simulate the fractionation process using shortcut distillation columns (DSTWU). In the example of three-component separation, two columns are needed; column 1 and column 2. Ensure that the recovery or purity are within the specification. If necessary, optimise the model to determine the optimum number of stages and reflux ratio.
2. Create a DWC flow sheet by combining four RADFRAC model blocks with two splitters as in Figure 2.
3. Set the rectifying column (section A) stage number as $2/3$ of the total number of stages of column 1.
4. Set stripping column (section D) stage number as $2/3$ of the total number of stages of column 2.
5. Set the pre-fractionation column (section B) stage number as the sum of the remaining stages in columns 1 and 2.
6. Set number of stages of middle column (section C) equal to that of the pre-fractionation column (section B).
7. Set the distillate flow rate of rectifying column (section A) based on distillate flow rate of column 1 in Step 1.

8. Set the distillate flow rate of middle section based on distillate flow rate of column 2 in Step 1.
9. Set feed stream location at the middle of the pre-fractionation column (section B) whereas set the middle stream location at the middle of middle column (section C) as well.
10. Set the reboiler duty at 70% of the total duties of columns 1 and 2 in Step 1. Alternatively, one can set the bottom flow rate based on bottom flow rate of column 2 in Step 1.
11. Set vapour and liquid splits equal to 0.5.
12. Run the model (*i.e.*, simulate DWC). If there is any error or non-convergence, fine tune the values in Steps 3 to 9.

Simulation of the customised DWC model is more difficult due to the complex interactions between different blocks with several recycle loops and interconnected streams in addition to the increased DOF. This leads to lack of proper initialisation and therefore prone to convergence error. Moreover, using four-column configuration requires extensive computational effort and simulation experience will help in converging the DWC model flow sheet. Hence, setting the key variables and parameters such as distribution and number of stages in each of the column sections, reflux ratio, liquid and vapour splits to each side of the dividing wall, feed stage locations and side draw locations is crucial to ensure convergence. Based on our experience, the following approaches can be used to minimise the convergence issues. First is changing the RADFRAC algorithm to Newton or quasi-Newton or Broyden method due to their good convergence properties. Maximum iterations can be increased with appropriate error tolerance value, *i.e.* $1.0\text{e-}07$. To increase the model robustness, upon convergence, the initial values for temperature, liquid and vapour mole flows and mole fractions can be generated using the convergence option in the RADFRAC block. It is reasonable to select manipulated variables based on their sensitivity on the desired specifications. Our recent work (Othman *et al.*, 2015) indicates that reflux ratio has major effect on distillate purity, and reboiler duty heavily affects middle and bottom purities.

Optimisation

Part three of the approach involved optimisation. Parametric optimisation method was adopted in the work by varying the operating variables of the distillation block and evaluate the objectives variable values whilst maintaining the product specification. For distillation column design, minimum ratio of reflux flow rate requires infinite number of stages, while minimum number of stages which requires infinite reflux. It is known that

increasing the number of stages increases the capital cost whereas increasing the reflux ratio increases the operating cost due to more material being recycled and reheated in the reboiler and re-condensed in the condenser. Consequently, there is a trade-off: larger columns have a larger upfront cost but lower operating costs, while smaller columns have smaller capital costs but are more expensive to operate. To obtain an initial optimum design, [column number of stages (N) \times reflux ratio (RR)] *vs.* N was plotted (Aspen Plus, 2012) using DSTWU model block in Case 1. This plot is a curve with a distinct minimum, where the economic optimum between the capital and operating cost trade-off often occurs. This basic heuristic essentially puts equal weight on the number of stages and reflux ratio. In essence, the argument is that a real column will need slightly more stages to achieve the separation modelled in the DSTWU block because a real column cannot achieve the same efficiency as the model. The optimum results from Case 1 such as number of stages, reflux ratio and feed stage would be used as initial input parameters for Case 2. Parametric optimisation was performed on Case 2 where feed stage location was varied to minimise the reboiler duty. Feed stage and middle output stream in Case 3 were also optimised for minimal reboiler duty. Note that, for Case 2 and Case 3, the design specification option in RADFRAC model blocks were used to maintain the desired purity of 99 wt% by manipulating the reflux ratio.

Analysis

Economic and environmental assessment. The last part of the work flow is the analysis; capital cost (CAPEX), operating cost (OPEX) as well as environmental performance would be calculated for Cases 2 and 3, and then compared. In addition, hydrodynamic and thermal analysis would be performed for Case 3. In process development, economic performance is the most assessed and important attribute for evaluating its feasibility for the continuation of process development. Usually in early design stages, economic feasibility is estimated with accuracy range of +30% to -20%. Although results from such preliminary evaluation may not accurately reflect the final profitability of a chemical plant, they can be used for comparison of several process alternatives. A single distillation column in Case 2 followed the typical sizing and costing of a single tower with a reboiler and a condenser. Overall, Case 2 had four towers, four reboilers and four condensers. For Case 3, a slightly different approach was used to calculate the cost of DWC. Since a single DWC is divided into four different sections, the cost is equivalent to the total cost of four separate towers with a reboiler and condenser. Alternatively, one may also determine the tower

cost by finding the diameter and height of a single tower required for the four sections. This is likely to give a lower estimate compared to the estimate based on cost of four towers with a reboiler and condenser. Hence, the latter is used in the present study for a conservative estimate. Overall, Case 3 has two dividing wall columns namely DWC1 and DWC2, with eight towers, two reboilers and two condensers in total.

The column diameter for equipment cost calculation was determined using the packing sizing option in Aspen Plus. The column was designed as a packed column with packing factor of 72 m^{-1} . For all stages, a height equivalent of theoretical (HETP) of 0.3 m was assumed. All columns were operated under vacuum condition between 10 to 40 mbar. Pressure drop was not considered at this stage. The column temperature must not exceed 270°C to prevent product degradation and must not cross the reboiler utility temperature profile. Material of construction (MOC) of all towers were carbon steel with stainless steel cladding and stainless steel packing. All rectifying sections have stainless steel demisters. The utility for condenser was cooling water whereas high pressure steam was used for reboiler utility. The utility data was based on Aspen Plus. For condenser cooling water, the inlet temperature is 20°C and outlet temperature is 25°C . The price is $\text{USD } 2.12\text{e-}07 \text{ kJ}^{-1}$ with minimum temperature approach of 5°C . High pressure steam was used for reboiler; the inlet temperature is 250°C in vapour phase while the outlet temperature is 249°C in liquid phase. The energy price is $\text{USD } 2.5\text{e-}06 \text{ kJ}^{-1}$ with minimum temperature of 5°C . Heat exchanger design and sizing for pre-heaters, reboilers and condensers were performed using the exchanger design and rating tools in Aspen Plus. The condensers were classic TEMA BEM type shell and tube exchangers, while the reboilers were kettle type heat exchanger. MOC for all reboilers and condensers were stainless steel since FA is highly corrosive. Aspen Plus and CAPCOST software (Turton *et al.*, 2008) were used to calculate capital cost. The chemical engineering plant cost index (CEPCI) value used is 603.1 for the year 2018.

The environmental analysis in this work focuses on CO_2 emissions. Malaysia has put an aim to voluntarily reduce by 40% its carbon emissions intensity of GDP (gross domestic product) by the year 2020 compared to 2005 levels (Othman and Masoud, 2014). The CO_2 is used as reference to measure the global warming potential (GWP). The larger the GWP, the more that a given gas warms the earth compared to CO_2 over that time period (US EPA, 2017). The most popular standards used for reporting CO_2 equivalents of streams are IPCC SAR, IPCC AR4 and US EPA (2009). In Aspen Plus, Carbon Tracking tools in the Utilities set-up option can be used to calculate the amount of CO_2 emitted

during the production process from burning of fuel source such as natural gas, coal and liquefied petroleum gas (LPG). The results provide guidance on the relative impacts of different types of products or industries with respect to resource use and emissions throughout the production line (Demire, 2015). The calculation of CO₂ was based on the CO₂ emission factor data sources or user defined values. The former can be obtained from the European Commission Decision of 2007/589/EC (2007) or US Environmental Protection Agency Rule of E9-5711 (2009). In this study, the latter was selected as the CO₂ emission factor data source and natural gas was selected as the fuel source. In Aspen Plus, the corresponding Prop-Set properties is CO₂E-US. Note that, the CO₂ analysis in this work only involved the production of high pressure steam for heating utility. The economic and environmental comparisons were based on the following equation:

$$\% \text{ Diff.} = \left(\frac{C_{\text{DWC}} - C_{\text{CDC}}}{C_{\text{DWC}}} \right) \times 100\% \quad \text{Equation (1)}$$

Here, C is the economic or environmental assessment value. Note that negative value means savings achieved by DWC compared to CDC.

Hydraulic analysis of DWC – effect of packing type.

Although dividing wall columns are economically viable, industry avoided investment in these columns for many years in the past. One of the reasons is the lack of understanding of the effect of the dividing wall (Schultz *et al.*, 2002; Kaibel *et al.*, 2006). Therefore, it is important to understand the hydrodynamic behaviour of DWC, *i.e.* pressure drops, flooding points, vapour and liquid flows, which depend on column diameter and column internals such as packing selection. The estimation of maximum hydraulic capacity and pressure drop for a given packing is particularly important to prevent operational and control problems (Barroso-Muñoz *et al.*, 2010), and can be used for design purposes (Uresti-Melendez and Rocha, 1993). In addition, hydraulic analysis produces plot for flow rates versus stage, and they can be used to identify and eliminate column bottlenecks. In Aspen Plus, hydraulic analysis is available in the tray/packing rating option. Tray/packing rating allows user to specify the column section diameter and packing/tray details. Accordingly, the model calculates performance and hydraulic information such as flooding, downcomer back-up and pressure drop. The advantage of four-column configuration is the flexibility to determine the column diameter and internal configuration of DWC. Thus, the size of each column section can be customised explicitly. However, working with customised DWC models raised a serious pressure gradient issues due the use of four interconnected blocks. To ensure correct column pressure

gradient, we suggest the following procedure to set up the column pressure.

1. Set all top column section pressures as well as splitters as equal with no pressure drop as in Equations (2) and (3). Run the model. See Figure 4 for the four column sections of a DWC.

$$P_{A_{N=n}} = P_{B_{N=1}} = P_{C_{N=1}} = P_{D_{N=1}} \quad \text{Equation (2)}$$

$$P_{M1} = P_{M2} \quad \text{Equation (3)}$$

Here, $P_{A_{N=n}}$ is the pressure at the bottom stage of column section A. The $P_{B_{N=1}}$, $P_{C_{N=1}}$ and $P_{D_{N=1}}$ is the pressure at the top stage of column sections B, C and D, respectively. The P_{M1} and P_{M2} is the pressure the splitters.

2. Upon convergence, select the update pressure profile option for rectifying column section A, and run the simulation.
3. Once converged, use the pressure of the last stage of section A as the pressure for liquid splitter (M1) and top pressure of pre-heater section (B) and middle section (C), as in the following equation. Click the update pressure profile option and run the simulation.

$$P_{A_{N=n}}^{\text{New}} = P_{M1} = P_{B_{N=1}} = P_{C_{N=1}} \quad \text{Equation (4)}$$

4. Once converged, identify the highest bottom pressure between B and C. The highest pressure is used to set the vapour splitter (M2) pressure while the lowest is used to set the top pressure of stripping section (D) as shown in the following equations.

$$\text{IF}(P_{B_{N=n}}^{\text{New}} > P_{C_{N=n}}^{\text{New}}) \quad \text{Equation (5)}$$

$$\text{THEN}(P_{M2} = P_{B_{N=n}}^{\text{New}}) \text{ AND } (P_{D_{N=1}} = P_{C_{N=n}}^{\text{New}}) \quad \text{Equation (6)}$$

$$\text{ELSE}(P_{M2} = P_{C_{N=n}}^{\text{New}}) \text{ AND } (P_{D_{N=1}} = P_{B_{N=n}}^{\text{New}}) \quad \text{Equation (7)}$$

5. Run the simulation. It is advisable to perform the analysis from the rectifying section (A) and go downward to the stripping section (D). With some practice, the above procedure could help to achieve positive pressure gradient inside the column. Transfer function block was used to automatically update the pressure as described in the procedure. The hydraulic analysis in this work is used to study the effect of different packing on column economics. Decreasing the column diameter for constant mass flow rates gives higher flow rates of liquid and gas per unit area, which results in higher pressure drops and larger pumping costs. Conversely, increasing the column diameter leads to larger equipment cost. Thus, there will be an economic optimum diameter depending upon relative costs and the relation between pressure drop and flow rates.

For hydraulic analysis, the column diameter used was based on packing sizing option in Aspen

Plus with increment of 0.15 m, the calculated diameter was rounded up to nearest 0.15 m (Premkumar and Rangaiah, 2009) whereas HETP was varied from 0.1 m to 0.7 m. Top column pressure was fixed at 40 mbar and 10 mbar for DWC1 and DWC2, respectively. Packing rating option was used with updated pressure drop profile along the column using built-in vendor correlations. After simulating the model with the new HETP values, the pressure profile was updated before simulating again. This was to ensure the results were based on the updated pressure profile. Two types of structured packing in the Mellapak series were evaluated, namely, 125Y and 250Y. During simulation, the product specifications and bottom stream temperature were monitored. While maintaining the product specifications, the bottom stream temperature must not cross the reboiler utility temperature. Temperature cross is best avoided as the productivity of a heat exchanger will be significantly reduced. In Aspen Plus, convergence warning will be issued for temperature cross situation in heat exchangers.

The column economics is performed by plotting total DWC packing cost (TC_{DWC}) + operating cost against F-factor. The packing cost is mainly driven by material price and packing area; in addition, 30% to 50% is added for manufacturing. To calculate the packing cost, $C_{packing}$, Equation (8) was adopted whereas Equation (9) was used to calculate the total packing cost, TPC of column n . The total packing cost for DWC, TPC_{DWC} , is the summation of TPC of all columns in each of two dividing wall columns as in Equation (10).

$$C_{packing} = \left[\left(\frac{A_{packing}}{2} \right) T_{packing} \rho_{moc} C_{moc} \right] \gamma_{mc} V_{vessel} \quad \text{Equation (8)}$$

$$TPC^n = C_{packing} \cdot V^n \quad \text{Equation (9)}$$

$$TPC_{DWC} = \sum_n TPC^n \quad \text{Equation (10)}$$

Here, $A_{packing}$ is the packing area ($m^2 m^{-3}$), $T_{packing}$ is the sheet thickness (m), ρ_{moc} is the material density ($kg m^{-3}$), C_{moc} is material cost (USD kg^{-1}), V is the column volume (m^3) and γ_{mc} is the manufacturing cost between 30%-50%. Material of construction is based on stainless steel. The ρ_{moc} is taken as 8000 $kg m^{-3}$ whereas C_{moc} is assumed USD 2 kg^{-1} while γ_{mc} was considered 50%. For calculation of column volume, V the diameter is the same for all packing type. The operating cost was based on reboiler and condenser energy consumption using the same data as in the economic assessment.

RESULTS AND DISCUSSION

Simulation Results

Figure 5 shows the plot of N^*RR vs. N for PC, LC, MC and HC columns. The economic optimum occurs

around the minimum of the N^*RR vs. N graph. For PC, LC, MC and HC columns, the optimum stage was at stages 29, 27, 24 and 9 with reflux ratio of 1.077, 1.326, 1.876 and 0.028, respectively. These values were then used in the design of Case 2. Sensitivity analysis was performed to determine optimal feed location of all dividing wall columns for Case 2 as shown in Figures 6a to 6d. The simulation results of Case 2 were then used as initial design variable for Case 3. Using the design steps described in the DWC design section, the process was modelled using two dividing columns connected in series. To get the desired purity, reflux ratio, reboiler duty and liquid split were varied accordingly. The sensitivity analysis of feed stream location to reboiler and condenser duty for each DWC was performed. The results are shown in Figures 6e and 6f.

Selected simulation results for Cases 2 and 3 are shown in Table 3. There is a significant difference in the number of stage in which DWC has a larger number of stages per unit compared to conventional distillation column (CDC). This is expected due to the number of components separated in a DWC column. The temperature profiles of both DWC1 and DWC2 are shown in Figure 7 whereas Figure 8 shows the composition profiles for both DWC1 and DWC2. The temperature difference at the divided section (B and C) is due to the effect of feed stream and different liquid/vapour split flow to the divided section. The top product of DWC1 was a mixture of C6, C8 and C10, C12 was fractionated in the middle product stream of the middle column, and the remaining components were taken out as the bottoms and fed to DWC2. The top product of DWC2 was C14 whereas C16, C18, C18:1 and C18:2 were the middle product stream, and bottom product mostly contains TG. Note that, the generation of the temperature and composition profile were based on underlying material, equilibrium, summation and energy equation systems. For example, one of the main parameters involved in composition profile is phase equilibrium and selecting suitable

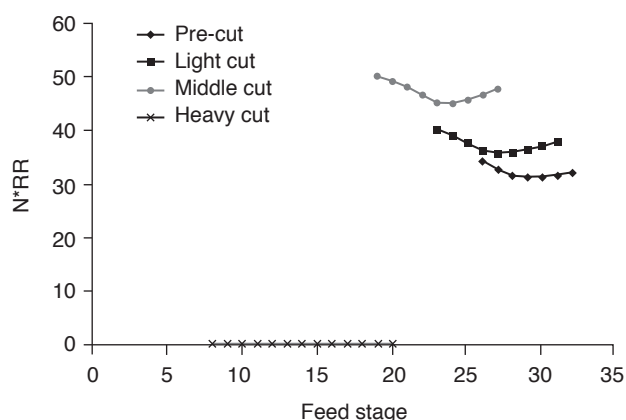


Figure 5. Simulation results for optimal number of stages.

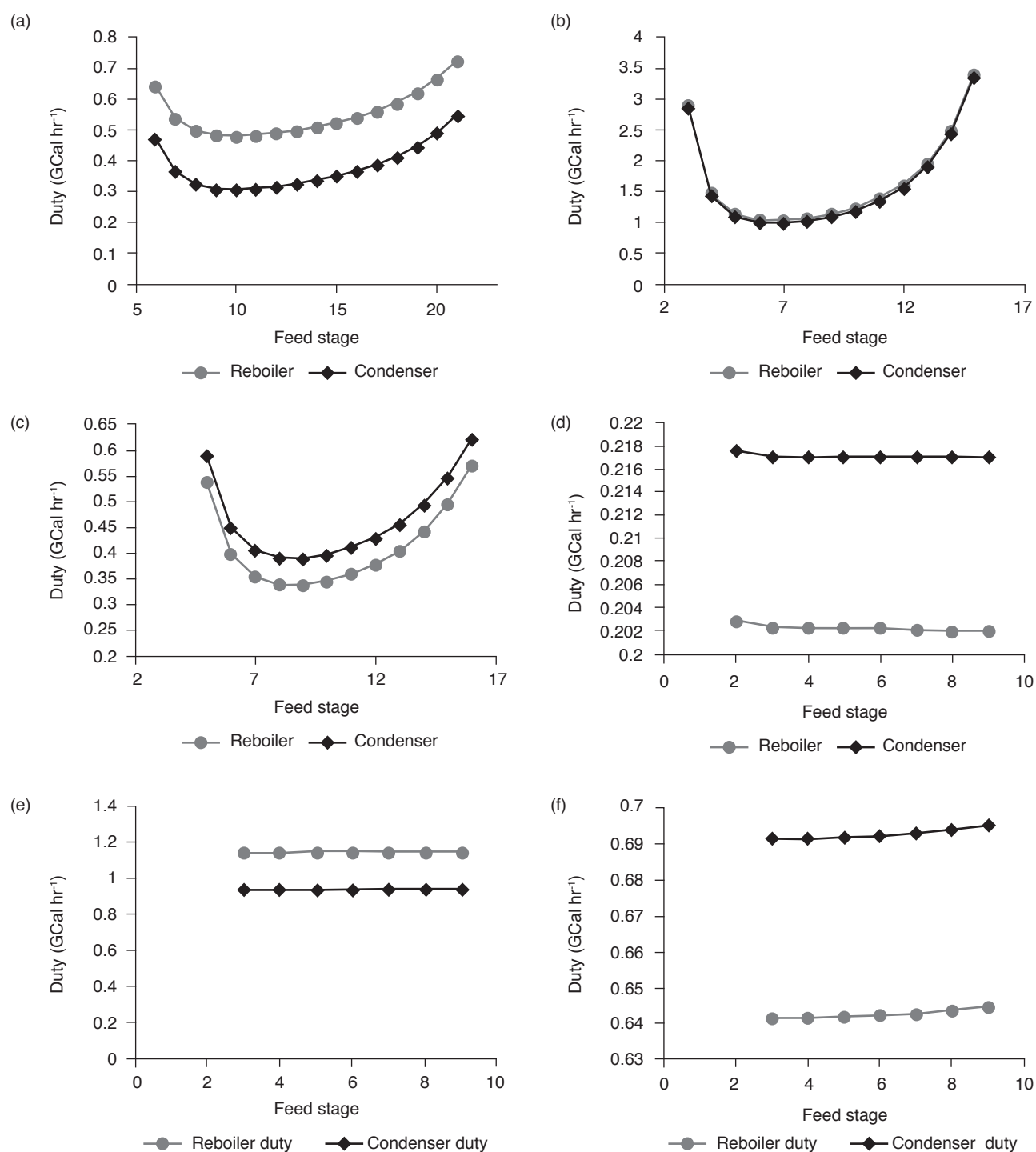


Figure 6. Results for reboiler and condenser column duties for (a) pre-cut, (b) light cut, (c) middle cut, (d) heavy cut, (e) DWC 1 and (f) DWC 2 as a function of feed stage location.

thermodynamic model for predicting phase equilibrium is crucial. Good selection will ensure good convergence as well as close to actual results. However, actual data were not available either in literature nor plant data for comparison and validation purposes. Nevertheless, we made an effort to make sure that the thermodynamic model was properly selected and validated to ensure the process was model and simulated correctly.

Economic and Environmental Comparison

Based on the methodology described in the Analysis Section, economic and environmental assessment were performed on Cases 2 and 3. The results are presented in Table 4. The total CAPEX for column tower in Case 3 was 12.5% higher than Case 2. This was mainly due to the higher tower and larger diameter of the DWC in Case 3 as shown in

TABLE 3. SUMMARY OF SIMULATION RESULTS

	Case 2				Case 3	
	PC	LC	MC	HC	DWC 1	DWC 2
Reflux ratio	3.45	1.48	2.16	0.1	12.7	4.5
Stages	29	27	24	9	10 (A) 11 (B) 11 (C) 18 (D)	11 (A) 11 (C) 18 (D) 6 (D)
Feed stage	10	7	9	5	5 (at B)	5 (at B)
Pressure (mbar)	40	40	15	10	40	15
Reboiler duty (kW)	556.4	1 186.5	402	252.6	1 332.2	746.7
Condenser duty (kW)	354.39	1 147.6	461.9	235.2	1 091.4	804.8
Distillate temp (°C)	153.5	197.1	194.9	211.9	153.5	194.8
Bottom temp (°C)	207.7	232.6	221.6	227.3	232.6	238.1
Diameter (m)	1.44	2.15	1.63	1.33	1.72 (A) 1.38 (B) 2.00 (D) 1.34 (C)	1.88 (A) 1.34 (C) 1.36 (B) 1.91 (D)

Note: A, B, C and D are the dividing wall column (DWC) sections for rectifying, pre-fractionation, middle and stripping respectively. PC - pre-cut. LC - light cut. MC - middle cut. HC - heavy cut.

Table 3. On the other hand, the bare module cost of reboilers and condensers for Case 3 was 16.8% and 7.3% lower than that in Case 2, respectively. Overall, the bare module cost of Case 3 was 3.1% cheaper than Case 2. Nevertheless, major benefits of DWC can be seen in OPEX. DWC able to save 16.9% of cooling water cost and 10.2% of heating steam cost compared to CDC. This energy reduction leads to similar reduction in CO₂ emission at 10.2%. These results are aligned with DWC advantages for other applications (Serra *et al.*, 1999; Yildirim *et al.*, 2011). In process plants, this is a huge advantage since distillation consumes almost 40% of total plant energy consumption.

Hydraulic Analysis – Effect of Packing Type

Based on the methodology in the Hydraulic Analysis of DWC Section, the column diameter was rounded to the nearest 0.15 m. For DWC1, the column diameter for sections A, B, C and D were set to 1.75 m, 1.45 m, 1.45 m and 2 m, respectively. Whereas for DWC2, the column diameter for sections A, B, C and D were set to 1.9 m, 1.45 m, 1.45 m, and 1.9 m, respectively. The overall packing cost of different HETP and packing types are shown in Figure 9. Note that the column diameter was fixed for all cases. For all HETP values, Mellapak 250Y was the most expensive whereas Mellapak 125Y cost the least which was mainly due to the packing area. The performance of the packing does affect the OPEX. As shown in Figures 9b and 9c, for both packing types, the reboiler duty increases with increase in HETP. This is expected as increased

HETP increased the column height and pressure drop which leads to higher reboiler duty. The cooling duty also increased slightly with increase HETP due to higher reboiler duty which led to more vapour load to the rectifying section of the column. Overall, the total OPEX with inclusion of reboiler and condenser costs shows an increment with increased HETP for both packing types as shown in Figures 9b and 9c. The hydraulic analysis also shows the feasibility or convergence status of the column to meet the temperature specifications as well as fulfilling the minimum approach temperature and temperature profiles of reboiler heat exchangers. Table 5 shows the column reboiler convergence results. At HETP of 0.1 m, all packing types have good reboiler convergence. At HETP of 0.3 m, only Mellapak 125Y have good reboiler convergence for both DWC1 and DWC2. Overall, increased HETP and packing area lead to poor convergence of the column reboiler particularly for DWC2 due to the increased pressure drop column temperature which then affect the reboiler heat exchanger temperature utility profile.

CONCLUSION

This work outlines the modelling and simulation of two dividing wall columns, each using the four-column configuration, for FA fractionation into four products and residue. Our steady state rigorous simulations show the feasibility of the DWC for the given purification specifications. Total CAPEX shows a slight advantage of DWC over conventional

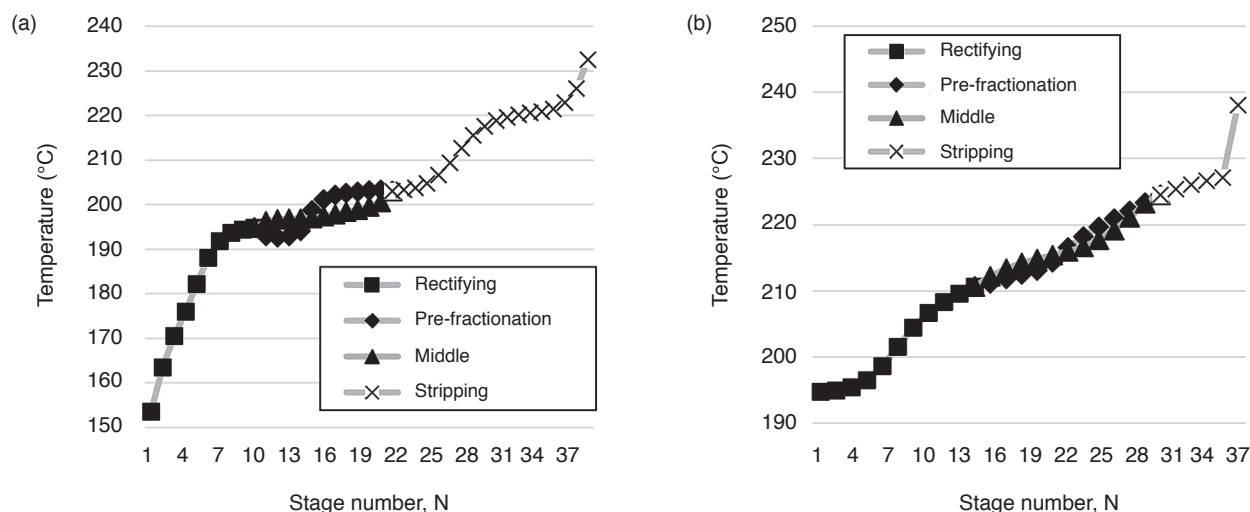


Figure 7. Temperature profile of (a) DWC1 and (b) DWC2.

TABLE 4. SUMMARY OF ECONOMIC AND ENVIRONMENTAL ANALYSIS

	Case 2	Case 3	Difference (k USD)	Difference (%)
Total bare module cost				
Column towers (k USD)	675.8	760.6	-84.8	-12.5
Condensers (k USD)	355.3	295.6	59.7	16.8
Reboilers (k USD)	1 364.7	1 264.9	99.8	7.3
Total (k USD)	2 395.9	2 321.1	74.8	3.1
Operating cost				
Cooling (k USD yr ⁻¹)	14.8	12.7	2.1	16.9
Heating (k USD yr ⁻¹)	257.6	233.9	23.7	10.2
Total (k USD yr ⁻¹)	272.5	246.6	25.9	10.5
Environmental analysis				
Total CO ₂ emission (kg hr ⁻¹)	773.04	701.7	-	10.2

Note: Positive difference means case 3 (DWC) are more economical.

DWC - dividing wall column.

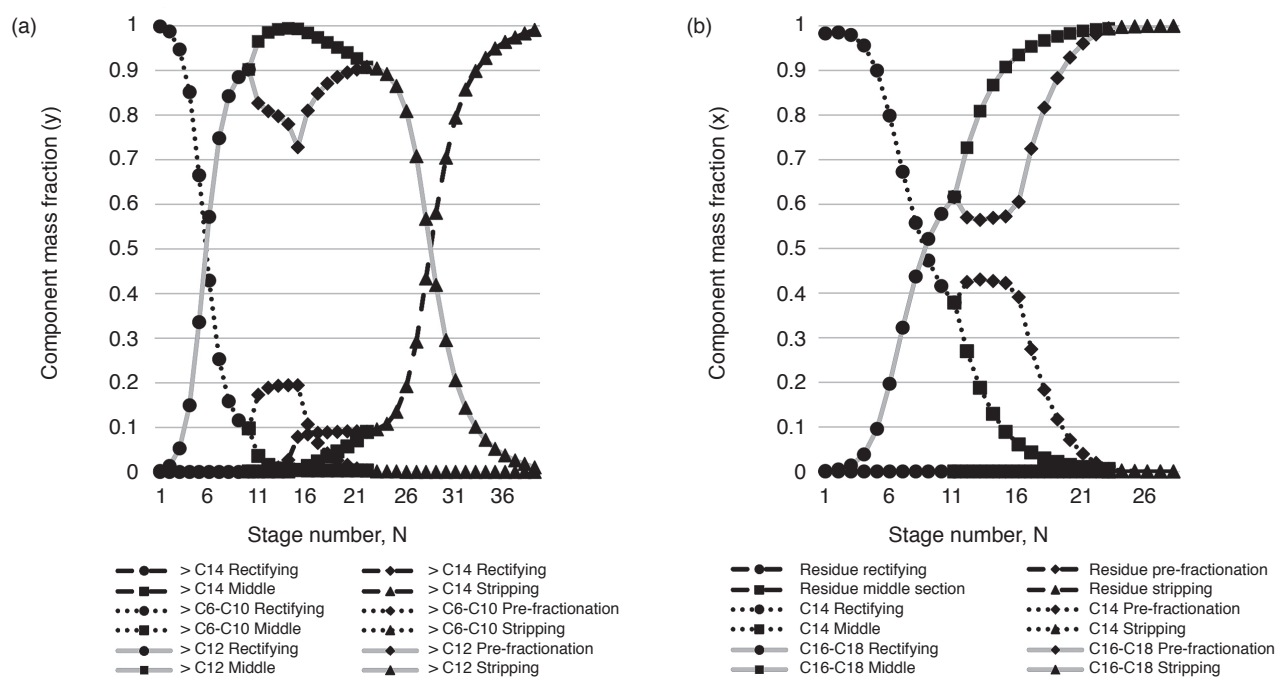


Figure 8. Vapour fraction composition profiles of (a) DWC1 and (b) DWC2.

TABLE 5. EFFECT OF PACKING TYPE AND HEIGHT EQUIVALENT OF THEORETICAL PLATE (HETP) TO COLUMN REBOILER CONVERGENCE

Packing type	HETP of DWC1					HETP of DWC2				
	0.1	0.2	0.3	0.5	0.7	0.1	0.2	0.3	0.5	0.7
125Y	A	A	A	A	A	A	A	A	B	B
250Y	A	A	A	A	B	A	B	B	C	C

Note: A - indicate that the column reboiler fully converged. B - indicate warning in which the minimum temperature approach of 5°C were violated. C - indicate error in which the reboiler temperature cross with the utility temperature.

DWC – dividing wall column.

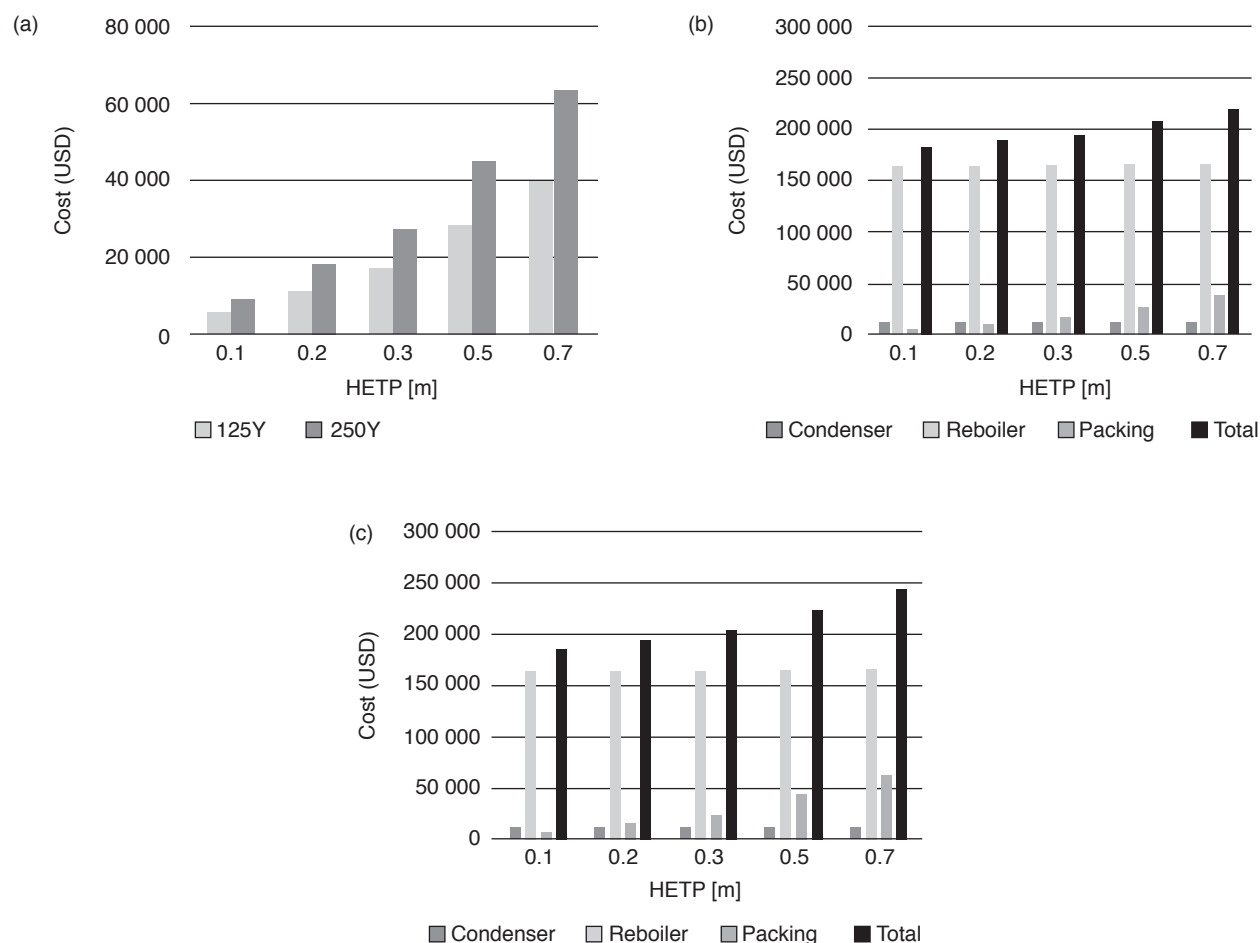


Figure 9. (a) Effect of height equivalent of theoretical plate (HETP) on cost of different Mellapak packing types, (b) operating cost for Mellapak 125Y, (c) operating cost for Mellapak 250Y. The operating cost for reboiler and condenser were based on annual cost.

distillation columns. However, the major advantage is in OPEX. Using DWC, 16.9% and 10.2% savings can be achieved on cooling and heating utilities as well as 10.2% of CO₂ emissions reduction. Hydraulic analysis of DWC was carried out through rigorous modelling utilising the packing rating option. Mellapak 125Y series provides the most feasible option based on the overall economic performance and operation of reboiler convergence. Overall, our study shows the feasibility of fractionating fatty acids in oleochemical industry using DWC. Our future work will focus on heat integration of dividing wall columns designed in this work

as well as on the installation of a mini-plant for operational and controllability studies of dividing wall columns.

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